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THREE-DIMENSIONAL MASS-CONSERVING ELEMENTS FOR COMPRESSIBLE FLOWS

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Abstract—A variety of finite-element schemes has been used in the numerical approximation of compressible flows, particularly in underwater acoustics. In many instances instabilities have been generated due to the lack of mass conservation. In this paper we develop new two- and three-dimensional elements which avoid these problems.

1. INTRODUCTION

It has been known for several years that many finite-element formulations of fluid flows have potentially serious instabilities (see e.g.[1–8]). A great deal of attention has been given to the incompressible case, and a variety of techniques for dealing with these instabilities has been developed. These include reduced integration[9], artificial diffusion[10], penalty methods[11] and the development of special stable elements[12–14], to cite only a few references in a very large literature. The special elements have proven to be of great practical value since they typically can be implemented by using standard elements in a Galerkin formulation and then applying various filtering techniques to the pressures computed from the latter.

The compressible case is similar in the sense that elements which are unstable for incompressible flows are also unstable in the compressible case. This has been analysed mathematically and shown to be equivalent to the failure of the Babuška–Brezzi angle condition between the finite spaces used in the formulation[3, 4]. On the other hand, the compressible case is dissimilar in that the angle condition is not sufficient for stability. Put differently, there are elements which perform quite satisfactorily for incompressible flows but which exhibit a number of instabilities in the compressible case. These are usually of secondary nature; i.e. they do not destroy the entire calculation, but they do lead to slower rates of convergence than normal and, hence, less accurate and less efficient approximations.

The key to these has been shown to be related to mass conservation[1, 4, 7]. In the incompressible case it is necessary to have mass conservation (i.e. a divergence-free velocity field) only in an appropriate averaged sense. For example, if linear elements are used to represent the fluid velocity u_h, typically one has

$$\int_T \operatorname{div} u_h = 0 \tag{1.1}$$

for each subdivision T defining the grid. This is different from

$$\operatorname{div} u_h = 0 \tag{1.2}$$

holding at each point, the latter being equivalent to exact mass conservation.

In the steady compressible case the relevant vector field is the mass flow u_h, and the assertion is that without (1.2) serious errors will occur in the approximation that do not exist in the incompressible case.

Fortunately, there are a number of mass-conserving elements that have been developed in the two-dimensional case. The most widely used are the second-order accurate union jack or crisscross element[3] and the first-order linear element developed by Thomas[14]. The goal of this paper is to develop analogous elements for three spatial dimensions. The analog of the Thomas element is given in Sec. 2, and the analog of the crisscross element is given in Sec. 4. In Sec. 3 we give an apparently new element which, like the criss-cross element, is second-order accurate, but, like the Thomas element, does not have restrictive grid regularity conditions.

To describe these elements we consider the specific case of steady potential flow. We let φ denote the potential and ρ the density. The governing equations in the flow region Ω are

$$\operatorname{div} \rho \, \overrightarrow{\operatorname{grad}} \, \varphi = 0 \quad \text{in } \Omega, \tag{1.3}$$

$$\varphi = \varphi_\Gamma \quad \text{on } \Gamma_D, \tag{1.4}$$

$$\overrightarrow{\operatorname{grad}} \, \varphi \cdot n = v_n \quad \text{on } \Gamma_N. \tag{1.5}$$

On one part of the boundary of Ω, namely Γ_D, the potential φ_Γ is given, and on the other, Γ_N, the normal velocity v_n is given. The density ρ and velocity $\overrightarrow{\operatorname{grad}} \, \varphi$ are related through Bernoulli's equation.

Galerkin formulations typically work in terms of the mass flow

$$u = \rho \, \overrightarrow{\operatorname{grad}} \, \varphi, \tag{1.6}$$

since jump conditions across a shock are equivalent to the continuity of u and, thus, are an intrinsic part of the formulation. Entropy conditions ruling out expansion shocks, on the other hand, are introduced through modifications of the density ρ. The formulation consists of a finite-element space $\mathcal{V}_h$ in which the mass flow is represented and a finite space $\mathcal{S}_h$ for the potential. The parameter $h > 0$ denotes a generic mesh spacing. One seeks a u_h in $\mathcal{V}_h$ and a φ_h in $\mathcal{S}_h$ such that

$$\int_\Omega \frac{u_h \cdot v^h}{\rho} + \int_\Omega \varphi_h \operatorname{div} v^h = \int_{\Gamma_D} \varphi_\Gamma \, v^h n, \tag{1.7}$$

$$\int_\Omega \operatorname{div} u_h \, \psi^h. \tag{1.8}$$

The approximate mass flow u_h is required to satisfy

$$u_h \cdot n = u_n \quad \text{on } \Gamma_N, \tag{1.9}$$

where u_n is the given normal mass flow, and (1.7) holds for all v^h in $\mathcal{V}_h$ whose normal components are zero on Γ_N. Equation (1.8), on the other hand, holds for all ψ^h in $\mathcal{S}_h$, the boundary condition (1.4) being natural in this formulation. Once a basis for $\mathcal{V}_h$ and $\mathcal{S}_h$ has been selected, (1.7)–(1.8) reduced to a system of nonlinear equations, the nonlinearity coming from the functional dependence of the density ρ on the mass flow u_h.

In the next three sections we shall display pairs $\mathcal{V}_h, \mathcal{S}_h$ which satisfy exact mass conservation (1.2). In each of these cases this property is a direct consequence of the following inclusion property[3]:

$$\mathcal{S}_h = \operatorname{div} [\mathcal{V}_h], \tag{1.10}$$

That is, each element ψ^h is a divergence $\operatorname{div} v^h$ of some v^h in $\mathcal{V}_h$, and conversely. Indeed, suppose (1.10) were true for the pair $\mathcal{S}_h$, $\mathcal{V}_h$. Then if u_h is the mass flow arising from (1.7)–(1.8), we have $\operatorname{div} u_h \in \mathcal{S}_h$. Thus, letting $\psi^h = \operatorname{div} u_h$ in (1.8) we get

$$\int_\Omega (\operatorname{div} u_h)^2 = 0,$$

and hence (1.2) holds.

The inclusion property (1.10) is the primary vehicle in the paper for constructing mass-conserving elements. In the next two sections, $\mathscr{S}_h$ is taken as a suitable space of piecewise constant functions, and $\mathscr{V}_h$ is constructed so that (1.10) holds. In the last section the converse is used. Here $\mathscr{V}_h$ is taken as a suitable space of piecewise linear functions, and $\mathscr{S}_h$ is defined by (1.10).

Each of the spaces introduced in the next sections also satisfies the Babuška–Brezzi angle condition. The proofs will be omitted since they are very close to the two-dimensional proofs and quite technical in nature.

2. A FIRST-ORDER ELEMENT

We suppose for simplicity that Ω is a polygonal region in $\mathbf{R}^3$, and we subdivide into tetrahedral elements $T_1, \ldots, T_n$. The space $\mathscr{S}_h$ consists of all piecewise constant functions on this grid. Thus, $\mathscr{S}_h$ has n degrees of freedom, and a local basis $\psi_1, \ldots, \psi_n$ is defined in the standard manner; i.e.

$$\psi_j(T_l) = \begin{cases} 1 & \text{if } j = l, \\ 0 & \text{if } j \neq l. \end{cases} \tag{2.1}$$

To define $\mathscr{V}_h$ we use the reference tetrahedron T_{ref} shown in Fig. 1. In particular, we consider incomplete linear functions in T_{ref} having the form

$$v = \alpha + \beta\xi. \tag{2.2}$$

The four degrees of freedom α, β are uniquely determined by specifying the normal component $v \cdot \nu$ at the centroid m of each of the four faces S. The space $\mathscr{V}_h$ will consist of images of these functions.

More precisely, let T_j be a tetrahedron in the grid and consider the affine mapping

$$\sigma_j : T_{\mathrm{ref}} \longrightarrow T_j. \tag{2.3}$$

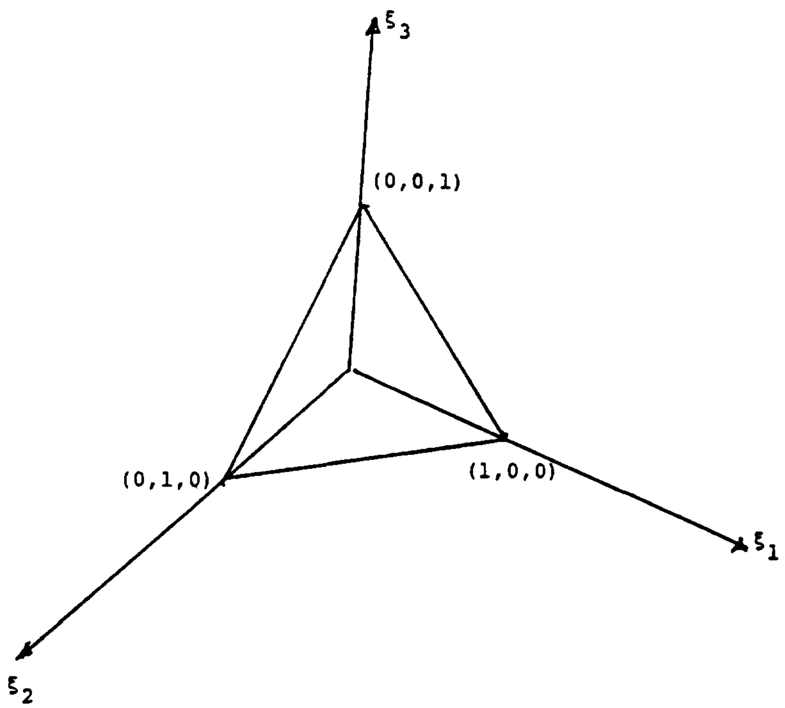

Fig. 1. T_{ref}.

Then functions v_h in $\mathcal{V}_h$ have the following form in T_j:

$$v_h(\sigma_j(\xi)) = \alpha + \beta\xi. \tag{2.4}$$

The parameters α, β are determined by specifying $v \cdot \nu$ at the centroid of each face.

Suppose $\{F_1, \ldots, F_N\}$ is the set of all faces, and let m_j be the centroid of F_j, with ν_j being a unit normal to F_j. Then $\mathcal{V}_h$ has N degrees of freedom, and any v_h in $\mathcal{V}_h$ is uniquely determined by specifying

$$v_h \cdot \nu_j(m_j) \quad (j = 1, \ldots, N). \tag{2.5}$$

A basis $\phi_1, \ldots, \phi_N$ for $\mathcal{V}_h$ is obtained by requiring that

$$\phi_j \cdot \nu_l(\mathrm{m}_l) = \begin{cases} 1/|F_j| & \text{if } j = l, \\ 0 & \text{if } j \neq l, \end{cases} \tag{2.6}$$

where $|F_j|$ is the area of F_j. Observe that since $\phi_j \cdot \nu_l$ is linear on F_j,

$$\int_{S_l} \phi_j \cdot \nu_l = \begin{cases} 1 & \text{if } j = l, \\ 0 & \text{if } j \neq l. \end{cases} \tag{2.7}$$

Moreover, ϕ_j is identically zero in any T_l which does not contain F_j as a face; i.e. $\phi_1, \ldots, \phi_N$ is a locally defined basis.

Functions v_h in $\mathcal{V}_h$ are not necessarily continuous, but they are square integrable and have a square integrable divergence. In fact, for each tetrahedron T,

$$\operatorname{div} v_h = \frac{1}{|T|}\int_T \operatorname{div} v_h = \frac{1}{|T|}\int_{\partial T} v_h \cdot \nu \quad \text{in } T, \tag{2.8}$$

where $|T|$ denotes the volume of T, and ν is the outer normal. This is the only regularity required on the variational principle (1.7)–(1.8). These elements, however, cannot be used for the incompressible case, since continuity is required there.

We assert that the inclusion property (1.10) holds for this pair of spaces. Since v_h is linear, div v_h is a piecewise constant and hence is in $\mathcal{S}_h$. We must show that every function ψ_h has this form. To see this we first select the function v satisfying

$$\operatorname{div} v = \psi_h \quad \text{in } \Omega. \tag{2.9}$$

Using the basis ϕ_j, let

$$v_h = \sum_{j=1}^{N}\left(\int_{F_j} v \cdot \nu_j\right)\phi_j. \tag{2.10}$$

Observe that for any T_l,

$$\operatorname{div} v_h = \frac{1}{|T_l|}\int_{T_l} \operatorname{div} v_h = \frac{1}{|T_l|}\int_{\partial T_l} v_h \cdot \nu. \tag{2.11}$$

But using (2.7) and (2.10), we have

$$\int_{\partial T_l} v_h \cdot \nu = \int_{\partial T_l} v \cdot \nu = \int_{T_l} \operatorname{div} v. \tag{2.12}$$

In light of (2.9) we therefore have

$$\operatorname{div} v_h = \frac{1}{|T_l|}\int_{T_l} \operatorname{div} v_h = \frac{1}{|T_l|}\int_{T_l} \psi_h = \psi_h \tag{2.13}$$

in T_l. Since ψ_h is an arbitrary function in $\mathcal{S}_h$, it follows that (1.10) must hold.

Incidently, the Babuška–Brezzi angle condition requires that, in addition to (2.13), v_h must satisfy

$$\|v_h\|_0 + \|\operatorname{div} v_h\|_0 \leq C\|\psi_h\|_0, \tag{2.14}$$

where

$$\|v\|_0 = \left\{\int_\Omega |v|^2\right\}^{1/2}, \tag{2.15}$$

and $0 < C < \infty$ is uniformly bounded independent of the grid. This can be verified directly from (2.10) once explicit formulas are obtained for the basis $\phi_1, \ldots, \phi_N$. This calculation is similar to the one in [14], and it does require that the grid be quasiregular in the sense that the ratios of the maximum side length to the diameter of each T are uniformly bounded.

Functions in $\mathcal{V}_h$ are capable of only first-order accuracy. The reason for this can be seen from (2.2). The first component v_1 of v does not contain terms involving ξ_2 and ξ_3. Hence, $v_h \in \mathcal{V}_h$ is not a complete piecewise linear function.

Since $\mathcal{S}_h$ contains only piecewise constant functions, it too is capable of only first-order accuracy. Thus, if u_h and φ_h are the approximations obtained from (1.7)–(1.8), then

$$\|u - u_h\|_0 \leq Ch\,\|\operatorname{grad} u\|_0, \tag{2.16}$$

$$\|\varphi - \varphi_h\|_0 \leq Ch\,\|\operatorname{grad} \varphi\|_0, \tag{2.17}$$

where h is the maximum diameter of tetrahedrons T_l.

3. A SECOND-ORDER ELEMENT

In many applications it is important to have second-order approximations to the mass flow and velocities. To achieve this we use the same grid as in Section 2 but with a larger space $\mathcal{V}_h$. The idea is to increase the size of

$$\mathcal{V}' = \{v_h : \operatorname{div} v_h = 0\}, \tag{3.1}$$

so that the inclusion property (1.10) is not affected.

Indeed, we retain the same notation introduced in Section 2, and, as before, let $\mathcal{S}_h$ denote the space of piecewise constant functions. To define $\mathcal{V}_h$ we let $F_1, \ldots, F_N$ denote the faces of the tetrahedrons with $m_1, \ldots, m_N$ being the associated centroids. With each face F_j we select a normal ν_j along with two independent tangential directions $\tau_j^{(1)}, \tau_j^{(2)}$. A function v_h is in $\mathcal{V}_h$ if and only if

(i) v_h is a linear polynomial in each T_j;
(ii) v_h is continuous at each centroid m_j.

In the previous section functions v_h were required only to have a continuous normal component at the centroids m_j ($j = 1, \ldots, N$). Here all three components of v_h are continuous. Moreover, the representation of v_h in each T_j is in terms of a complete linear polynomial.

As in the last section v_h in $\mathcal{V}_h$ are not necessarily continuous everywhere in Ω. They are, however, square integrable with square integrable divergences. Moreover,

$$\operatorname{div} v_h = \frac{1}{|T|}\int_{\partial T} v_h \cdot \nu \tag{3.2}$$

holds for each tetrahedron T.

Observe that $\mathcal{V}_h^{*}$ has $3N$ degrees of freedom, and a locally defined basis $\phi_1^{(i)}, \ldots, \phi_N^{(i)}$ $(i = 0, 1, 2)$ can be selected so that for $j = 1, \ldots, N$ we have

$$\phi_j^{(0)} \cdot \nu_l(m_l) = \begin{cases} |F_l| & \text{if } j = l, \\ 0 & \text{if } j \neq l, \end{cases} \tag{3.3}$$

$$\phi_j^{(0)} \cdot \tau_l^{(t)}(m_l) = 0, \quad l = 1, \ldots, N, \; t = 1, 2, \tag{3.4}$$

and, for $i = 1, 2$,

$$\phi_j^{(i)} \cdot \nu_l(m_l) = 0 \quad \text{all } l, \tag{3.5}$$

$$\phi_j^{(i)} \cdot \tau_l^{(t)}(m_l) = \begin{cases} |F_l| & \text{if } i = t \text{ and } j = l, \\ 0 & \text{otherwise.} \end{cases} \tag{3.6}$$

Note that since $\phi_j^{(i)}$ is a linear function on the faces F_l, we have

$$\int_{S_l} \phi_j^{(0)} \cdot \nu_l = \begin{cases} 1 & \text{if } j = l, \\ 0 & \text{if } j \neq l, \end{cases} \tag{3.7}$$

$$\int_{S_l} \phi_j^{(0)} \cdot \tau_l^{(t)} = 0 \quad \text{all } l, t, \tag{3.8}$$

and, for $i = 1, 2$,

$$\int_{S_l} \phi_j^{(i)} \cdot \nu_l = 0 \quad \text{all } l, \tag{3.9}$$

$$\int_{S_l} \phi_j^{(i)} \cdot \tau_l^{(t)} = \begin{cases} 1 & \text{if } j = l \text{ and } i = t, \\ 0 & \text{otherwise.} \end{cases} \tag{3.10}$$

Thus any v_h in $\mathcal{V}_h^{*}$ can be written as

$$v_h = \sum_{j=1}^{N}\left(\int_{S_j} v_h \cdot \nu_j\right)\phi_j^{(0)} + \sum_{j=1}^{2}\sum_{j=1}^{N}\left(\int_{S_j} v_h \cdot \tau_j^{(i)}\right)\phi_j^{(i)}. \tag{3.11}$$

It follows from (3.2) and (3.9) that the second sum in (3.11) is divergence free. It therefore does not play a role in the inclusion property (1.10), but it does contain the extra terms (missing in the space defined in Section 2) giving second-order accuracy.

To verify (1.10) for this case we select a function v satisfying (2.9) and let

$$v_h = \sum_{j=1}^{N}\left(\int_{S_j} v \cdot \nu_j\right)\phi_j^{(0)} \tag{3.12}$$

(i.e. the divergence-free part is omitted). Equations (2.11)–(2.13) remain valid, and, hence, as before we have

$$\operatorname{div} v_h = \psi_h \quad \text{in } T. \tag{3.13}$$

Assuming the grid is quasiregular in the sense cited in Section 2, one can directly verify the angle condition introduced in [3]. A consequence is second-order accuracy; i.e.

$$\|u - u_h\|_0 \leq Ch^2 \, \|D^2 u\|_0 \tag{3.14}$$

is obtained for the mass flow. Since $\mathcal{S}_h$ consists only of piecewise constant elements, first-order accuracy [i.e. (2.17)] is the best we can obtain for the potential φ. However, the results in [3] indicate that φ_h is a second-order accurate approximation to the average $1/|T| \int_T \varphi$ in each tetrahedron T.

4. THE THREE-DIMENSIONAL CRISS-CROSS ELEMENT

Let Ω be a rectangular domain in $\mathbf{R}^3$, divided into $m_1 m_2 m_3$ cubes B_α, where $\boldsymbol{\alpha} = (i, j, k)$ $(0 \leq i < m_1, 0 \leq j < m_2, 0 \leq k < m_3)$, by a uniform grid of mesh spacing h. We denote the corners of the cubes by ω_{ijk}, centers by $\omega_{i+1/2, j+1/2, k+1/2}$, and the center of each face by $\omega_{i+1/2, j+1/2, k}$, $\omega_{i, j+1/2, k+1/2}$ or $\omega_{i+1/2, j, k+1/2}$.

Each cube is partitioned into 24 congruent tetrahedrons by considering divisions along the four diagonals of each cube, the two diagonals of each face of the cube, and the three lines joining the centers of opposite faces of the cube (Fig. 2). We number the faces of each cube from 1 to 6, as shown in Fig. 3. Each of these six faces of the cube will contain the basis of four tetrahedrons. We can now identify any tetrahedron in the grid by $T_\alpha^{r,s}$, where $\boldsymbol{\alpha} = (i, j, k)$ gives the cube in which the tetrahedron is contained, $1 \leq r \leq 6$ specifies the face on which the base is located, and $1 \leq s \leq 4$ specifies the tetrahedron completely.

Let $\mathcal{V}_h^*$ be the space of all $\mathbf{R}^3$-valued continuous functions over Ω which are piecewise linear for each tetrahedron. We take our approximate space $\mathcal{V}_h$ to be that subspace of $\mathcal{V}_h^*$ in which the nodes at the centers of the faces of each cube are condensed out. This is done by specifying the value at such a node to be the average of the values at the four vertices of the face. More precisely, for $v_h = \sum_{l=1}^{3} v^l \mathbf{e}_l$‡ $\in \mathcal{V}_h^*$,

$$\begin{aligned} v^l(\omega_{i+1/2, j+1/2, k}) &= v^l_{i+1/2, j+1/2, k} \\ &= \frac{1}{4} \sum_{q=0}^{1} \sum_{p=0}^{1} v^l_{i+p, j+q, k}, \quad l = 1, 2, 3. \end{aligned} \tag{4.1}$$

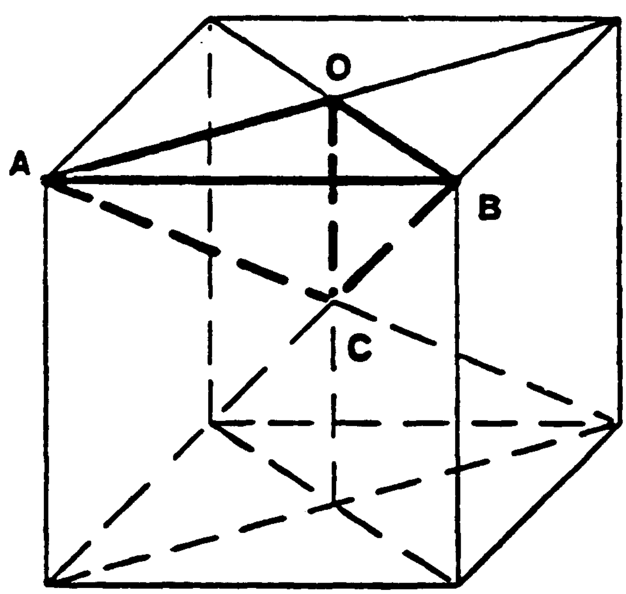

Fig. 2.

‡$\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ form an orthonormal basis for $\mathbf{R}^3$.

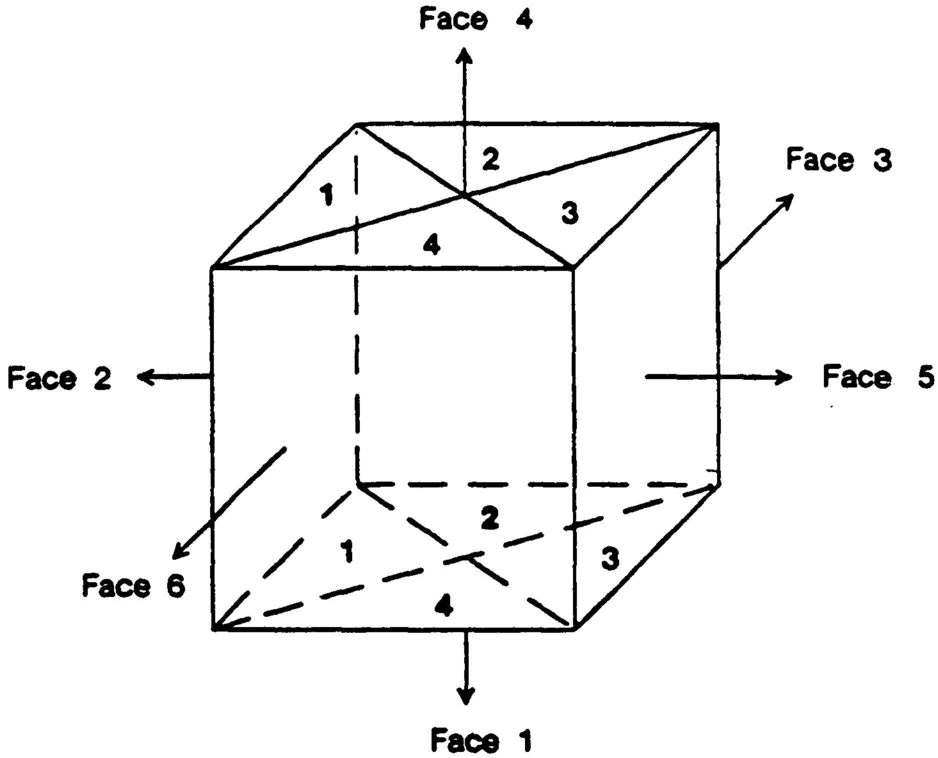

Fig. 3.

The numbers $v^l(\omega_{i+1/2,j,k+1/2})$ and $v^l(\omega_{i,j+1/2,k+1/2})$ will be similar averages.

The dimension of $\mathcal{V}^h$ is equal to $3N$, where N, the number of unconstrained nodes, is given by $(m_1 + 1)(m_2 + 1)(m3 + 1) + m_1m_2m_3$. Let $\mathcal{N}$ be the set of all nodes (constrained or unconstrained). For every node ω_α, define a function $\phi_\alpha \in \hat{\mathcal{V}}_h$ by

$$\phi_\alpha(\omega_\beta) = \delta_{\alpha\beta} = \begin{cases} 1 & \text{if } \alpha = \beta, \\ 0 & \text{if } \alpha \neq \beta. \end{cases}$$

Then any function $\hat{\mathcal{V}}^h_h$ in $\hat{\mathcal{V}}^h_h$ can be represented as $v^h = \sum_{l=1}^3 (\sum_{\alpha\in\mathcal{N}} v^l_\alpha \phi_\alpha)\mathbf{e}_l$. For a function in $\mathcal{V}_h$ the coefficients for constrained nodes are replaced by suitable averages.

Let $\mathcal{S}_h$ be the set of functions that are constant over each tetrahedron. $\phi^{r,s}_\alpha$ will denote the value of ϕ in $T^{r,s}_\alpha$. Define $\mathcal{S}_h$ to be the set of $\phi \in \mathcal{S}_h$ such that, for any α,

$$\text{(i) } \phi^{r,1}_\alpha + \phi^{r,3}_\alpha = \phi^{r,2}_\alpha + \phi^{r,4}_\alpha \quad (r = 1, \ldots, b), \tag{4.2}$$

$$\text{(ii) } \sum_{S=1}^{4} (\phi^{r,s}_\alpha + \phi^{r+3,s}_\alpha) = C_\alpha, \quad \text{a constant} \quad (r = 1, 2, 3). \tag{4.3}$$

With this choice of $\mathcal{S}_h$ and $\mathcal{V}_h$, we have $\mathcal{S}_h = \operatorname{div} [\mathcal{V}_h]$, as proved in the Appendix.

Moreover, our proof also shows that the Babuška–Brezzi condition is satisfied, so that for every $\phi \in \mathcal{S}_h$, we can find a $w \in \mathcal{V}_h$ satisfying

$$\operatorname{div} w = \phi \quad \text{in } \Omega, \quad \|w\|_0 \leq C\|\phi\|_{-1},$$

where $0 < C < \infty$ is bounded independently of the grid.

The second-order-accurate space of functions that are lienar over each B_α is easily seen to be a subspace of $\mathcal{V}_h$. Similarly, the space of functions constant over each B_α is a subset of $\mathcal{S}_h$.

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APPENDIX

We now prove the following theorem:

THEOREM

For the spaces $\mathcal{V}_h$ and $\mathcal{M}_h$ mentioned in Sec. 4, we have $\mathcal{M}_h = \text{div}\,[\mathcal{V}_h]$.

Moreover, for any $\phi \in \mathcal{M}_h$, we can find a $w \in \mathcal{V}_h$ satisfying

$$\text{div}\, w = \phi \quad \text{in } \Omega, \quad \|w\|_0 \leq C\|\phi\|_{-1}. \tag{A1}$$

Proof. Let $\phi = \text{div}\,\vec{v}$, where $\vec{v} \in \mathcal{V}_h$. Referring to Fig. A.1 and denoting $\phi_\alpha^{1,s}$ by ϕ_s, we have

$$\phi_1 = \frac{v_A^1 - v_O^1}{h} + \frac{2v_B^2 - v_A^2 - v_O^2}{h} + \frac{2v_O^3 - 2v_B^3}{h}.$$

Similarly,

$$\phi_2 = \frac{2v_B^1 - v_O^1 - v_E^1}{h} + \frac{v_E^2 - v_O^2}{h} + \frac{2v_C^3 - 2v_B^3}{h},$$

$$\phi_3 = \frac{v_D^1 - v_E^1}{h} + \frac{v_D^2 + v_E^2 - 2v_B^2}{h} + \frac{2v_C^2 - 2v_B^3}{h},$$

$$\phi_4 = \frac{v_D^1 + v_A^1 + 2v_B^1}{h} + \frac{v_D^2 + v_A^2}{h} + \frac{2v_C^3 - 2v_B^3}{h}.$$

From this we see that

$$\phi_1 + \phi_3 = \phi_2 + \phi_4 = \frac{v_A^1 + v_D^1 - v_O^1 - v_E^1}{h} + \frac{v_D^2 + v_E^2 - v_O^2 - v_A^2}{h} + 4\,\frac{v_C^3 - v_B^3}{h}. \tag{A2}$$

This proves (4.2) for the function ϕ in the case $r = 1$. The other cases can be verified similarly. We now prove (4.3)

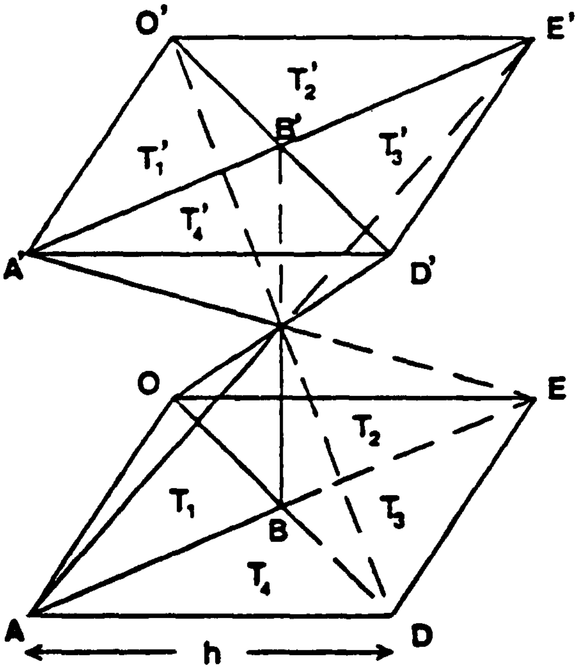

Fig. A.1. Sample tetrahedron.

for ϕ. We use ϕ_s and ϕ_s' to denote $\phi_\alpha^{s,s'}$, respectively. By calculations similar to the ones above we obtain

$$
\begin{aligned}
\frac{1}{8}\sum_{s=1} (\phi_s + \phi_s') &= \frac{(v_A^1 + v_{A'}^1 + v_D^1 + v_{D'}^1) - (v_O^1 + v_{O'}^1 + v_E^1 + v_{E'}^1)}{4h} \\
&+ \frac{(v_D^2 + v_{D'}^2 + v_E^2 + v_{E'}^2) - (v_A^2 + v_{A'}^2 + v_O^2 + v_{O'}^2)}{4h} \\
&+ \frac{(v_{A'}^3 + v_{O'}^3 + v_{E'}^3 + v_{D'}^3) - (v_A^3 + v_O^3 + v_E^3 + v_D^3)}{4h} \\
&= D_x v^1 + D_y v^2 + D_3 v^3 = \mathrm{div}_h\, v|_\alpha .
\end{aligned}
\tag{A3}
$$

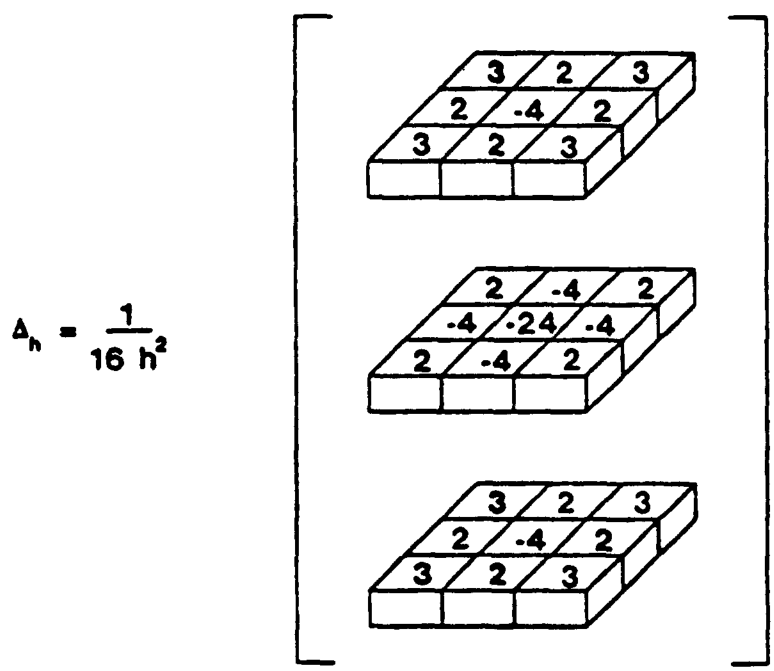

Fig. A.2.

We have used averaging expressions for v_B^3 and $v_{B'}^3$ above. By the symmetry of the expression for $\mathrm{div}_h v$, it follows that the same result must be obtained for $r = 2$ and $r = 3$—i.e. (4.3) holds. Hence, $\phi \in \mathcal{M}_h$—i.e. $\mathrm{div}[\mathcal{V}_h] \subset \mathcal{M}_h$. Now, let $\phi \in \mathcal{M}_h$. We will find $v \in \mathcal{V}_h$ satisfying (A3), which we rewrite as

$$\mathrm{div}_h v|_{i,j,k} = \bar{\phi}|_{i,j,k}. \tag{A4}$$

Here, the left side stands for the expression

$$\begin{aligned} &\frac{1}{4h}\sum_{q=0}^{1}\sum_{p=0}^{1}\{(v^1_{i+1,j+p,k+q} - v^1_{i,j+p,k+q}) \\ &\quad + (v^2_{i+q,j+1,k+p} - v^2_{i+q,j,k+p}) + (v^3_{i+p,j+q,k+1} - v^3_{i+p,j+q,k})\} \\ &\quad = D_x v^1|_{i,j,k} + D_y v^2|_{i,j,k} + D_z v^3|_{i,j,k}. \end{aligned} \tag{A5}$$

The right side equals $1/h^3\int_{B_{ijk}}$. Using (A2), we can obtain the value of v^3 at the central node as

$$\begin{aligned} v^3_{i+1/2,j+1/2,k+1/2} &= \frac{h}{4}[\phi^{1,2}_{i,j,k} + \phi^{1,4}_{i,j,k}] \\ &\quad - \frac{1}{4}\sum_{p=0}^{1}\{(v^1_{i+1,j+p,k} - v^1_{i,j+p,k}) \\ &\quad + (v^2_{i+p,j+1,k} - v^2_{i+p,j,k}) + (v^3_{i+p,j,k} + v^3_{i+p,j+1,k})\}. \end{aligned} \tag{A6}$$

Similar formulas hold for the other components of v at the central node of B_α. We shall use (A4) to determine v at the corner nodes and then define v at central nodes by (A6). To solve (A4), we introduce a discrete potential $\{\theta_{i+1/2,j+1/2,k+1/2}\}$, constant over each box $B_{i,j,k}$ and satisfying

$$\begin{aligned} v^1_{i,j,k} &= \frac{1}{4h}\sum_{q=0}^{1}\sum_{p=0}^{1}(\theta_{i+1/2,j-1/2+p,k-1/2+q} - \theta_{i-1/2,j-1/2+p,k-1/2+q}) \\ &= (G^h_x\theta)_{i,j,k}, \end{aligned} \tag{A7}$$

$$\begin{aligned} v^2_{i,j,k} &= \frac{1}{4h}\sum_{q=0}^{1}\sum_{p=0}^{1}(\theta_{i-1/2+q,j+1/2,k-1/2+p}\ \theta_{i-1/2+q,j-1/2,k-1/2+p}) \\ &= (G^h_y\theta)_{i,j,k}, \end{aligned} \tag{A8}$$

$$\begin{aligned} v^3_{i,j,k} &= \frac{1}{4h}\sum_{q=0}^{1}\sum_{q=0}^{1}(\theta_{i-1/2+p,j-1/2+q,k+1/2} - \theta_{i-1/2+p,j-1/2+q,k-1/2}) \\ &= (G^h_z\theta)_{i,j,k}. \end{aligned} \tag{A9}$$

Then (A4) implies that θ satisfies the following discrete Poisson equation:

$$\Delta_h\theta = (D_x G^h_x\theta + D_y G^h_y\theta + D_z G^h_z\theta)|_{i,j,k} = \bar{\phi}|_{i,j,k},$$

where Δ_h is the discrete Laplacian shown in Fig. A2. (Δ_h is the same as the "one-point quadrature stencil" described in Ref. [15].)

The equation above only involves θ at the centers of boxes. Since all boundary conditions are natural, we can extend the grid to cover Ω, and let $\theta_{i+1/2,j+1/2,k+1/2}$ be zero for points outside Ω. We now show that such a θ exists.

$$\text{Let } \Delta_h\psi = f \text{ in } \Omega \quad \text{and} \quad \psi = 0 \text{ outside } \Omega. \tag{A10}$$

(Here f is constant over each box $B_{i,j,k}$.) Then multiplying both sides by ψ and performing a discrete integration by parts, we obtain

$$-\left\{\{\sum_{(i,j,k)\in\Omega}(G^h_x\theta)^2_{i,j,k} + (G^h_y\theta)^2_{i,j,k} + (G^h_z\theta)^2_{i,j,k}\right\} = \sum(f\theta)_{i+1/2,j+1/2,k+1/2}.$$

Put $f \equiv 0$. Then, since $\theta = 0$ outside Ω, by starting from a corner of Ω and working through Ω, we see that $\theta \equiv 0$ in Ω. Hence, by the Fredholm alternative, (A10) has a unique solution for each f. We therefore obtain a solution for (A4). Defining v^1, v^2, v^3 by (A7)–(A9), we get the standard estimate

$$h^3\sum_{l=1}^{3}\sum_{(i,j,k)\in\Omega}\left|v^l_{i,j,k}\right|^2 \le C\|\phi\|_0^2 \tag{A11}$$

for some absolute constant $0 < C < \infty$. In addition, defining v at the centers of boxes by (A6), we obtain

$$h^2\sum_{l=1}^{3}\sum_{(i+1/2,j+1/2,k+1/2)\in\Omega}\left|v^l_{i+1/2,j+1/2,k+1/2}\right|^2 \le C^2\{\|\phi\|_{-1}^2 + h^2\|\phi\|_0^2\}.$$

Letting $\vec{v}$ be the continuous piecewise linear function whose value at each node is defined as above, we get

$$\sum_{i=1}^{3} \|v^i\|_0^2 \le C\{\|\phi\|_{-1}^2 + h^2\|\phi\|_0^2\} \quad \text{and} \quad \operatorname{div} \vec{v} = \phi.$$

Finally, using the inverse inequality for the uniform grid on Ω, we obtain, for $\phi \in \mathcal{M}_h$,

$$\|\phi\|_0 \le Ch^{-1}\|\phi\|_{-1}$$

This proves the theorem.